

2-Propanol-1,1,1-d3
84809-71-2 | DTXSID30480715

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 2.74 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.97e-01

Confidence level: 6.71e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1-Propanol</div> <div>Measured: 3.02</div> <div>Predicted: 4.69</div>	<div>Image not found</div> <div>Ethanol</div> <div>Measured: 1.58</div> <div>Predicted: 2.24</div>	<div>Image not found</div> <div>Thioacetamide</div> <div>Measured: 6.03</div> <div>Predicted: 6.43</div>
<div>Image not found</div> <div>Ethyleneimine</div> <div>Measured: 6.03</div> <div>Predicted: 4.17</div>	<div>Image not found</div> <div>Acetic acid</div> <div>Measured: 1.00</div> <div>Predicted: 2.40</div>	